Bulletin of the Chemists and Technologists of Macedonia., Vol. **10**, No 1–2, pp. 45 – 48 (1991)

CODEN: GHTMDD – 186 ISSN 0350 – 0136

Manuscript received: November, 15-th 1991 UDC 548.32 : 541.486

Short Communication

PREDICTION OF LATTICE CONSTANTS IN TUTTON SALTS

Vladimir Petruševski and Slobotka Aleksovska

Institut of Chemistry, Faculty of Sciences, The "Kiril i Metodij" University
Arhimedova 5, 91000 Skopje, Makedonija

The unit cell volumes of some Tutton salt compounds were predicted by a previously introduced method [1]. *Combining the results of these predictions with the data (lattice constant ratios) obtained from morphological studies, we were able to predict the lattice constants with a high degree of significance.*

Key words:
Tutton salts; lattice constants

INTRODUCTION

In our previous paper [1] we were able to predict the unit cell volume of Tutton salt compounds (monoclinic crystals, the general formula of which is $M_2^{I}M^{II}(XY_4)_2 \cdot 6H_2O$), knowing only their composition. This has been done by use of multiple linear regression analysis in which the dependent variable ($V_{\text{unit cell}}$) was presented as a function of (1) the effective ionic radius of M^+ ion; (2) the effective ionic radius of M^{2+} ion; (3) the X–Y distance and (4) the electronegativity of Y atom. The following equation was obtained:

$$\frac{V}{\text{Å}^3} = 111.55 + \frac{167.62 \cdot R(M^+)}{\text{Å}} + \frac{228.90 \cdot R(M^{2+})}{\text{Å}} + \frac{200.73 \cdot R(X-Y)}{\text{Å}} - 55.40 \cdot E(Y) \qquad (1)$$

In the present paper, the predicted values of the unit cell volumes together with data from morphological studies (the angle β and the ratios $a:b:c = p:1:r$, where p and r are some real numbers) of different Tutton salt crystals [2], serve as a source for the prediction of the lattice constants.

CALCULATION AND RESULTS

Data (the ratios $p : 1 : r$) for sulphate, selenate and chromate Tutton salts were available from morphological studies [2]. The lattice constants for some of them were already known [3 – 18] and are used to check the accuracy of the prediction. The following equation is used:

$$V_{\text{predicted}} = p \cdot r \cdot b^3 \cdot \sin\beta \qquad (2)$$

The solution of this equation gives the value of b; a and c are then simply calculated as: $a = p \cdot b$; $c = r \cdot b$.

A computer program (written in BASIC) was used to evaluate the unit cell volume and the lattice constants. The input data were $R(M^+)$, $R(M^{2+})$ and $R(X–Y)$, as well as p, r and . The results are given in Table I.

As seen from Table I, the accuracy of the fit between the actual and predicted values of the lattice constants seems to be very good. This may also be judged from the graph in Fig. 1. The critical point in the calculation is the accuracy with which the $p : 1 : r$ – ratios are determined, i.e. the data obtained by morphological measurements. Therefore, this simple method may be used to make reliable estimate of the lattice constants in Tutton salts and probably (given enough data), in other large classes of isomorphous compounds.

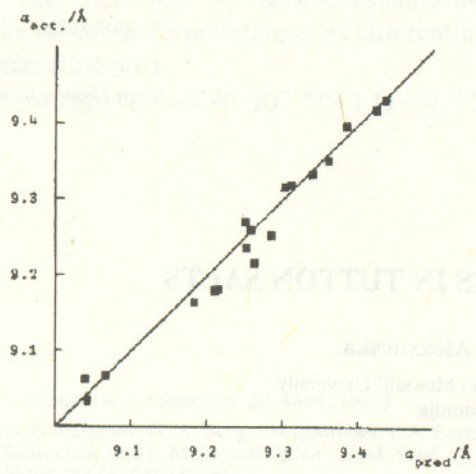

Fig. 1a

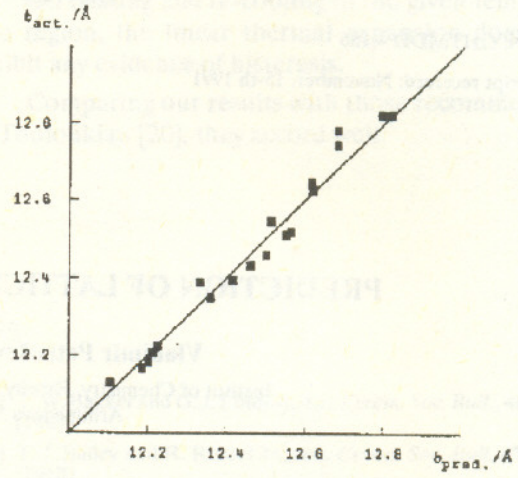

Fig. 1b

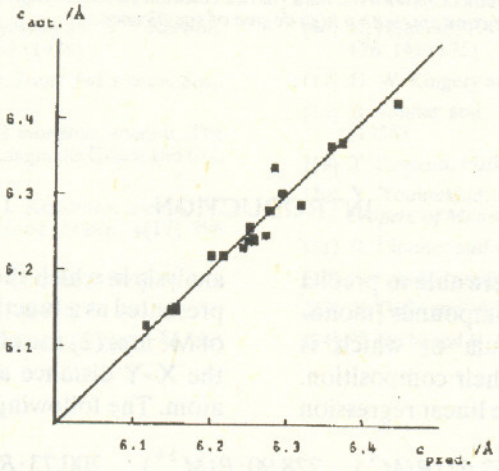

Fig 1 c

Figure 1. *Agreement between actual and predicted values of the unit cell axes, for some Tutton salts*

REFERENCES

[1] V. Petruševski and S. Aleksovska, *Croat. Chem. Acta* 64 (4), 577 (1991).

[2] A. N. Winchell and H. Winchell, *The Microscopic Characters of Artificial Inorganic Solid Substances. Optical Properties of Artificial Minerals*, Academic Press., New York, 1964.

[3] E. N. Maslen, K. J. Watson and F. H. Moore, *Acta Crystallogr.* B44, 102 (1988).

[4] N. W. Grimes, H. F. Kay and M. W. Webb, *Acta Crystallogr.* 16, 823 (1963).

[5] E. N. Maslen, K. J. Watson and F. H. Moore, *Acta Crystallogr.* C44, 1510 (1988).

[6] H. Montgomery and E .C. Lingafelter, *Acta Crystallogr.* 20, 728 (1966).

[7] H. Montgomery, R. V. Chastain and E. C. Lingafelter, *Acta Crystallogr.* 20, 731 (1966).

[8] H. Montgomery, R. V. Chastain, J. J. Natt, A.M. Witkowska and E. C. Lingafelter, *Acta Crystallogr.* 22, 775 (1967).

[9] P. G. Hodgeson, J. Whitnall, C. H. L. Kennard and F. H. Moore, *Cryst. Struct. Comm.* 4, 713 (1975).

[10] J. Whitnall, C. H. L. Kennard J. Nimmo and F. H. Moore, *Cryst. Struct. Comm.* 4, 717 (1975).

[11] D. J. Robinson and C. H. L. Kennard, *Cryst. Struct. Comm.* 1, 185 (1972).

[12] P. Hartman and C. F. Woensdregt, *Acta Crystallogr.* 17, 779 (1964).

[13] J. J. Van der Zee, K. G. Shields, A. J. Graham and C. H. L. Kennard, *Cryst. Struct. Comm.* 1, 367 (1972).

[14] K. G. Shields and C. H. L. Kennard, *Cryst. Struct. Comm.* 1, 189 (1972).

[15] K. G. Shields, J. J. Van der Zee and C. H. L. Kennard, *Cryst. Struct. Comm.* 1, 371 (1972).

[16] J. Whitnall, C. H. L. Kennard J. Nimmo and F. H. Moore, *Cryst. Struct. Comm.* 4, 709 (1975).

[17] H. Montgomery, *Acta Crystallogr.* B36, 440 (1980).

[18] A. Monge, E. Gutierez-Puebla, *Acta Crystallogr.* B37, 427 (1981).

Aknowledgement: The authors are indebted to Dr Ivan Grozdanov for his continuous interesr in the work

Table I. *Predicted values of lattice constants in some Tutton salts; where available, values obtained by diffraction are given for comparison. Standard abbreviations for the compound names are used (the chemical symbols for M^{I}, M^{II} and X; A– stands for ammonium, H – for hexahydrate).*

Compound	Actual				Predicted			
	$V/Å^3$	a/Å	b/Å	c/Å	$V/Å^3$	a/Å	b/Å	c/Å
ACuSH	691.6	9.216	12.398	6.301	695.5	9.263	12.417	6.295
ANiSH	682.7	9.181	12.459	6.239	688.8	9.214	12.502	6.251
AZnSH	691.0	9.236	12.514	6.246	697.2	9.252	12.553	6.273
ACdSH	727.6	9.433	12.823	6.286	732.4	9.436	12.820	6.320
AMnSH	716.5	9.398	123.742	6.256	712.3	9.385	12.683	6.253
AFeSH	704.3	9.32	12.65	6.24	703.9	9.312	12.618	6.259
ACoSH	690.6	9.254	12.521	6.244	698.0	9.285	12.565	6.257
KNiSH	646.8	8.985	12.167	6.128	647.6	8.993	12.186	6.117
KZnSH	654.3	9.034	12.184	6.148	656.0	9.042	12.202	6.150
KCuSH	655.0	9.066	12.13	6.149	654.3	9.066	12.104	6.158
KCoSH	657.8	9.061	12.207	6.151	656.8	9.039	12.215	6.156
RbCuSH	686.1	9.26	12.35	6.22	686.4	9.258	12.361	6.218
RbCoSH	683.4	9.180	12.433	6.230	688.9	9.210	12.463	6.244
CsCuSH	727.4	9.42	12.785	6.28	720.7	9.424	12.683	6.278
CsCoSH	726.7	9.316	12.824	6.365	723.2	9.302	12.795	6.359
TlCuSH	688.1	9.27	12.39	6.22	681.8	9.250	12.333	6.203
KCuSeH	690.6	9.165	12.224	6.336	686.4	9.183	12.227	6.285
ANiSeH	720.6	9.334	12.628	6.370	720.9	9.339	12.620	6.373
ACuSe	725.9	9.351	12.547	6.424*	727.6	9.361	12.515	6.445
RbMgSH					684.7	9.217	12.456	6.203
CsMgSH					719.0	9.304	12.780	6.326
TlMgSH					680.1	9.226	12.400	6.200
RbZnSH					688.0	9.188	12.466	6.246
CsZnSH					722.4	9.302	12.796	6.347
TlZnSH					683.4	9.206	12.424	6.225
RbCdSH					723.2	9.375	12.755	6.288
CsCdSH					757.6	9.477	13.054	6.409
RbMnSH					703.1	9.301	12.603	6.238
CsMnSH					737.4	9.400	12.930	6.349
TlMnSH					698.5	9.340	12.536	6.218
KFeSH					662.7	9.056	12.271	6.160
RbFeSH					694.7	9.227	12.503	6.256
CsFeSH					729.1	9.326	12.846	6.359
TlFeSH					690.2	9.260	12.463	6.230
TlCoSH					684.3	9.222	12.445	6.216
RbNiSH					679.6	9.130	12.422	6.236
CsNiSH					714.0	9.254	12.729	6.339
TlNiSH					675.1	9.170	12.392	6.192
KMgSeH					684.8	9,237	12.332	6.203
AMgSeH					726.0	9.430	12.709	6.316
RbMgSeH					716,8	9.346	12.596	6.311

Table I *(continued)*

Compound	Actual				Predicted			
	$V/Å^3$	$a/Å$	$b/Å$	$c/Å$	$V/Å^3$	$a/Å$	$b/Å$	$c/Å$
CsMgSeH					751.1	9.447	12.923	6.410
TlMgSeH					712.2	9.403	12.554	6.264
KZnSeH					688.1	9.202	12.335	6.254
AZnSeH					729.3	9.388	12.670	6.386
RbZnSeH					720.1	9.363	12.602	6.326
CsZnSeH					754.5	9.453	12.931	6.427
TlZnSeH					715.6	9.395	12.560	6.305
ACdSeH					764.5	9.549	12.869	6.473
AMnSeH					744.4	9.502	12.789	6.381
RbMnSeH					735.2	9.424	12.701	6.363
CsMnSeH					769.6	9.532	13.022	6.459
TlMnSeH					730.6	9.456	12.676	6.325
KFeSeH					694.8	9.270	12.376	6.237
AFeSeH					736.0	9.445	12.712	6.382
RbFeSeH					726.8	9.392	12.657	6.329
CsFeSeH					761.2	9.472	12.958	6.453
TlFeSeH					722.3	9.396	12.615	6.320
KCoSeH					688.9	9.262	12.316	6.232
ACoSeH					730.1	9.434	12.664	6.370
RbCoSeH					721.0	9.366	12.606	6.328
CsCoSeH					755.3	9.446	12.921	6.448
TlCoSeH					716.4	9.378	12.572	6.311
KNiSeH					679.7	9.182	12.292	6.220
RbNiSeH					711.8	9.312	12.584	6.330
CsNiSeH					746.1	9.388	12.878	6.426
TlNiSeH					707.2	9.337	12.516	6.283
RbCuSeH					718.5	9.376	12.501	6.338
CsCuSeH					752.8	9.509	12.850	6.399
TlCuSeH					713.9	9.397	12.479	6.302
AMgCrH					721.9	9.523	12.664	6.231
RbMgCrH					712.8	9.452	12.553	6.214
CsMgCrH					747.1	9.575	12.886	6.301

Резиме

ПРЕДВИДУВАЊЕ НА КОНСТАНТИТЕ НА ЌЕЛИИТЕ ВО ТУТОНОВИТЕ СОЛИ

Владимир Петрушевски , Слоботка Алексовска

Институт за хемија, Природно-математички факултет, Универзитет „Кирил и Методиј", Архимедова 5, 91000 Скопје, Македонија

Во нашиот претходен труд [1] ги предвидовме волумените на елементарните ќелии на некои Тутонови соли, користејќи статистички методи. Комбинирајќи ги резултатите од овие предвидувања со литературните кристалографски податоци (односи на параметрите на елеметарната ќелија), успеавме да ги предвидиме параметрите на елементарната ќелија. Резултатите од овие предвидувања се во добра согласност со експериментално добиените податоци за параметрите на елементарната ќелија